A NEW MONOCHROMATOR FOR HIGH HEAT LOAD SYNCHROTRON X-RAY RADIATION*

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Abstract

The high heat load associated with the powerful and concentrated x-ray beams generated by insertion devices (IDs) at a number of present and many of the future (planned or under construction) synchrotron radiation facilities poses a formidable engineering challenge for the design of monochromators and other optical devices.

Successful utilization of the intense x-ray beams from insertion devices depends critically on the development, design, and availability of optical elements that will provide acceptable performance under high heat load. Present monochromators can handle, at best, heat load levels that are an order of magnitude lower than those generated by these IDs. The monochromator described here, and referred to as the "inclined" monochromator, can provide a solution to the high heat load problem.

The inclined monochromator is different in a number of aspects from other conventional monochromators. Its primary differentiating characteristic is in the orientation of the diffracting planes. In the inclined geometry, the crystal surface normal and the normal to the diffracting crystal planes make an angle close to 90°. This leads to a number of interesting effects including spreading of the beam over a very large area (effectively reducing the incident heat flux), and also rendering a much smaller effective slope error. Thus, a substantial enhancement in the performance of the monochromator is realized. The preliminary results of a comparative numerical simulation of the performance of the inclined monochromator under the 5 kW power APS Undulator A beam are encouraging and provide a quantitative estimate of the expected enhancement.

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I. INTRODUCTION

The advent of insertion devices for the generation of dedicated and intense synchrotron x-ray beams has created a number of interesting engineering problems, particularly in the design of optical systems, that stem from the high head loads associated with these powerful beams.

A double crystal monochromator system is often used as the first optical element. The first crystal absorbs all but a narrow energy band of the photons from the white beam generated by the synchrotron sources. In many of the present synchrotron facilities, the beam power is in the few Watts range, requiring little or no cooling of the monochromator.

The power of the beams generated by insertion devices at a number of present facilities and many future facilities, such as the European Synchrotron Radiation Facility (ESRF) and the Advanced Photon Source (APS), can be higher by orders of magnitude. Active cooling of the monochromators is thus imperative. Wiggler beams have the highest total power but moderate power densities, while undulator beams have moderately high total power with very high power densities. From an engineering point of view, the combination of high total power and very high power density found in undulator beams poses the greatest challenge. Because the first crystal receiving the beam is distorted severely, far less photons than expected reach the experimentalists' sample. This is best illustrated by noting that, for a given source and monochromator system, one would expect an output photon count rate proportional to the storage beam current. A deviation from this linear relationship (marking onset of thermal distortion in the first crystal) occurs when further increases in the beam current (and thus in the thermal load) lead to smaller increases or even a decline in the photon count rate.[1]

This and related optical problems, collectively referred to as high heat load optics problems, have attracted considerable attention in the past several years[2] because utilization of the intense x-ray beams generated by insertion devices depends on the successful design of optical components capable of delivering the monochromatic beam to the experimental floor.

The design of a monochromator system that provides acceptable performance under the high heat load of the x-ray beams involves consideration of a number of factors. These include the material, thermal, structural, fluid mechanics, and diffraction aspects of the problem. Earlier efforts were aimed at efficient cooling of the first crystal so that the thermal gradient and, thus, the thermal strain in the crystal would be minimized. Liquid metal cooling has been a step in this direction, which, in combination with appropriately configured cooling channels in the crystal, can enhance the monochromator performance (as measured by photon count rate) by a factor of two or more compared with traditional water cooling.[3] Extensive numerical modeling for predicting the performance of monochromators has been carried out[4] that permits evaluation of various possible designs and optimization prior to fabrication and testing.

There have been other attempts at efficient cooling of the crystals, including jet and cryogenic cooling. From these and other studies and tests, a better understanding of the problem has emerged, bringing various aspects of the problem into sharper focus.

The overall design objective, however, should not be merely efficient cooling of the crystal but to devise and design a monochromator system that (consistent with operational requirements such as size, versatility, and ease of operation) has an acceptable and optimal performance as measured by the fraction of photons in the desired energy band width that reach the sample. The inclined monochromator described here resulted from an extensive examination of various possible design measured and aimed at achieving this overall objective. It fully exploits two of the options: (a) spreading the beam and (b) minimizing the slope error in a thermally unrelated way.

II. THE INCLINED MONOCHROMATOR

The double crystal inclined monochromator[5] consists of two single crystal blocks. The blocks are cut such that the normal to the diffraction planes of interest make a prescribed "inclined" angle β (close to 90°) with the crystal surface normal (Fig. 1). In conventional monochromators, β=0.

The incident beam in conventional monochromators is spread vertically on the first crystal due to the often shallow incident (Bragg) angles. In the inclined monochromator, the *horizontal* dimension of the beam footprint is also increased by a large factor. This magnification factor can be calculated using Fig. 2. The x-ray beam is incident at an angle θ_B on the surface of the inclined crystal represented by the P2 plane. The diffraction planes of interest are at an angle β with respect to this plane and are parallel to the P1 plane, as shown. In conventional monochromators, these planes coincide.

Assume that at normal incidence the beam has a rectangular footprint, and the height (in the vertical) and width (in the horizontal) of the footprint are v and h unit lengths, respectively. The beam footprint on a conventional crystal is increased by a factor of $1/\sin \theta_B$ due to spread in the vertical dimension.

The beam footprint on the surface of the inclined plane making an angle β with P1 is a long parallelogram. As seen, the height of the beam footprint is identical to that on the conventional crystal and equal to $v/\sin\theta_B$. The width of the footprint is evaluated as follows (see Fig. 2):

$$AG = EF = CD = v/\sin\theta_B \tag{1}$$

From triangles ABC and BCE, one obtains

$$AB = h/\cos\beta, \tag{2}$$

$$BC = h\tan\beta \tag{3}$$

and

$$BE = BC/\tan\theta_B = h\tan\beta/\tan\theta_B. \tag{4}$$

From triangle ABE, we have

$$AE = (h/\cos\beta)\sqrt{[1 + (\sin\beta/\tan\theta_B)^2]}, \tag{5}$$

and

$$\sin\gamma = 1/\sqrt{[1 + (\sin\beta/\tan\theta_B)^2]}. \tag{6}$$

The area of the inclined footprint is then

$$\text{Area} = (AG)(AE)\sin\gamma = vh/(\sin\theta_B\cos\beta). \tag{7}$$

Therefore, the beam footprint on the inclined crystal is larger than that on a conventional crystal by a factor of $1/\cos\beta$ (or by a factor of $1/(\sin\theta_B \cos\beta)$ larger than the normal incidence beam size.)

Fig. 3 plots the area magnification factor for the inclined crystals as a function of the angle of inclination, β, for Bragg angles of 2°, 5°, 10°, and 30°. It is seen, for example, that for an inclination of 85°, the area of the footprint is increased over 11 times, and thus the incident flux is reduced by a factor of 11.

This is one of the fundamental advantages of the present design. Because of the greatly reduced heat flux, a considerable reduction in the temperature of the crystal exposed to high heat load radiation is realized *with a substantially similar cooling method.* Lower temperatures lead to reduced thermal distortion when compared to a corresponding conventional x-ray monochromator. Also note that the inclined crystal not only leads to a *quantitative* increase in beam footprint size, but also to a *qualitative* spread of the beam in the form of an elongated footprint that may be advantageous from a heat transfer view point.

For any type of cooling scheme, but specially for cryogenic cooling in which a large cooling surface area is necessary, the larger beam footprint is very desirable. Due to the spread of the beam over a large surface area, the present design makes a several kW cryogenically cooled monochromator system feasible and more practical by (a) requiring far less vertical layers of cooling channels to provide the needed surface area for heat removal, thereby reducing the complexity in the design, (b) making the critical heat flux problem more manageable, (c) providing a more uniform temperature field on the surface and thus more efficient cooling, and (d) producing a lower overall temperature in the system leading to better cooling efficiency and reduced thermal strains. A conventionally cooled inclined crystal, however, is much simpler in design and operation, which is more desirable, and, of course, is more economical.

The second fundamental but distinct advantage of the inclined design is that *effective* slope errors are much smaller than in the case of conventional monochromators. Because of the orientation of the diffracting crystal planes with respect to the surface of the crystal, the thermal distortion of the crystal surface is only partially reflected in the slope error profile in the plane of scattering. The undesirable misorientation of the diffraction planes is considerably reduced. To clarify this point, consider the crystal shown in Fig. 1. We first note that pure bending of the crystal along its width will not affect the Bragg angle θ_B. For the bending along the length of the crystal, consider the case of $\beta \dashrightarrow 90°$. There is only a minor change in the Bragg angle θ_B as a result of this bend (which can be thought of as a major component of the thermal distortion in the crystal) because the crystal diffraction planes remain parallel. Now, as the inclination angle is decreased from 90° to 0° (conventional monochromators), the effect of such a bend will become progressively more pronounced. From this stand point, therefore, conventional monochromators are the worst designs.

Finally, it should be realized that the inclined crystal as outlined here is not an asymmetric crystal. Its inclined surface can be considered as the limit of a "stepped" crystal as the number of steps approach infinity (each step is a mini conventional crystal). Intuitively, therefore, the inclined crystal should function exactly like conventional symmetric crystals.

III. NUMERICAL SIMULATIONS

In order to examine the comparative performance of an inclined and a conventional monochromator, a simple numerical simulation of a model monochromator is carried out. To make a realistic case for the inclined crystal, the beam from the 2.5-m APS Undulator A is used as the radiation source. Specifications of this source are included in Table I.

The test monochromator system consists of two identical slabs of single crystal silicon. The first, which absorbs almost all the incident beam power, is thermally and structurally analyzed for various Bragg and inclination angles. The slope errors are computed and used as a comparative measure of the monochromator performance.

Table I: Data for the x-ray source and the monochromator used in the analyses.

X-ray source	APS Undulator A
Ring energy (GeV)	7
Beam current (mA)	100
Device length (m)	2.5
Deflection parameter	2.5
Vertical FWHM of the beam (mrad)	~0.073
Horizontal FWHM of the beam (mrad)	~0.36
Total beam power	5 kW
Peak power density	156 $kW/mrad^2$
Thermal filters	1.2-mm thick carbon
Windows	two 250-µm Be foils
Beam power at the monochromator	4.4 kW
Monochromator distance from the source	24 m
Peak normal incident flux at monochromator	~240 W/mm^2
Single crystal monochromator block	Si, 1-cm thick slab
Monochromator size	varies
Cooling area	back of monochromator
Coolant	10 ° C water
Heat transfer coefficient	1.0 W/cm^2-K
Thermal conductivity of Si 0°-130°C	1.7-1.0 W/cm-K
Young modulus (N/cm^2)	0.167×10^{10}
Poisson ratio	0.3
Coefficient of thermal expansion (K^{-1})	2.33×10^{-6}

The incident beam of about 5 kW power will have a total power of 4.4 kW after passing through the filter and beryllium (Be) window assemblies. Its non-uniform spatial profile is fully accounted for, and surface absorption is assumed in the computations

Because the incident Bragg and the inclination angles (and thus the beam footprint size) vary, the size of the monochromator is adjusted such that there is an unexposed margin of 0.5 cm on each side of the crystal. Diffraction is from the Si (111) planes, and the analysis is carried out for Bragg angles of 5.67° (20 keV) and 14.3° (8 keV) and inclination angles of 0°, 60°, 75°, and 85°.

Figure 4 shows a sketch of a typical model used in the numerical analyses with the heated area shaded. Actual models are much more detailed.

In the structural analyses of the crystal, at least six boundary conditions are needed to prevent rigid body motion. These are appropriately chosen such that the body is otherwise unconstrained. The displacements and the slope errors along the z-axis (shown in Fig. 4) are obtained in two coordinate systems. Both systems have their origins at the center of the exposed surface of the monochromator with one coincident axis. One system has its y-axis normal to the diffraction planes ($x_d y_d z_d$), while the other has its y-axis normal to the crystal surface ($x_s y_s z_s$). The $y_d z_d$ plane is a plane of scattering. The angle between $y_d z_d$ and $y_s z_s$ planes is the inclination angle.

Table II lists the maximum temperature differential and the maximum slope errors for the simulated cases. A considerable reduction in the maximum

Table II: Maximum temperature differentials in the first crystal and the maximum slope errors along the z-axes.

Bragg angle (°)	Inclination angle (°)	ΔT_{max} (°C)	Maximum slope error in $Y_s Z_s$ plane arc second	$Y_d Z_d$ plane arc second
5.67	0	1,735	690	690
5.67	60	517	360	215
5.67	75	184	160	70
14.3	0	2,960	870	870
14.3	60	1,240	430	245
14.3	75	570	220	85
14.3	85	157	72	11

temperature differentials from an (unrealistic value) of a few thousand °C to less than 200°C is observed as the crystal is inclined with respect to the incident beam. The significant reduction in the slope errors, particularly for large inclination angles, is another result of the inclined geometry. For a Bragg angle of 14.3° and an inclination angle of 85°, the slope error profiles along the z-axis in the xy planes of both the diffraction and surface coordinate systems are shown in Fig. 5. The rather modest maximum slope error of 11 arc seconds (for a maximum temperature differential of 157°C) is quite encouraging. Considering the crude (but adequate for this comparative study) model used here, it is expected that an optimally configured design, including an efficiently cooled system (using liquid gallium, for example,) will perform substantially better.

The main disadvantage of the inclined crystal may be its large size. However, it is quite possible to use an aperture so that a smaller monochromator, which still yields a high fraction of the expected photons, can be used. Other problems with fabrication and alignment should be expected, which, however, are not insurmountable.

IV. CONCLUSIONS

The simple model monochromatizing crystal used in the comparative analysis of the conventional and the inclined monochromators indicates that the inclined design can handle the intense radiation from future insertion devices. The radiation source used in this study is the APS Undulator A which constitutes the most difficult thermal load problem of all insertion devices planed for the next few years. An optimally designed and cooled inclined monochromator with an inclination angle of about 80° can provide a solution to the present high heat load optics problems. Plans have been underway at APS to construct and test a number of inclined monochromators. Some preliminary test results available at this time are very encouraging. These and the results of forthcoming tests, as well as the experience gained in the area of fabrication, alignment, and operation, will be published in forthcoming papers.

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1. R. K. Smither, G. A. Forster, D. H. Bilderback, M. Betzyk, K. Finkelstein, C. Henderson, J. White, L. E. Berman, P. Stefan, and T. Oversluizen, Rev. Sci. Instrum. **60**, 1486 (1989).

2. R. K. Smither and A. K. Freund, Editors, Worksop on High Heat Load X-ray Optics, Argonne National Laboratory, Argonne, Illinois, USA, **ANL/APS/TM-6** (1990).

3. A. M. Khounsary, T. M. Kuzay, P. J. Viccaro, D. M. Mills, and R. K. Smither, in Proc. of SPIE on X-Ray/EVU Optics for Astronomy and Microscopy, San Diego, California, USA, **1160** 145 (1989).

4. A. M. Khounsary, J. J. Chrzas, D. M. Mills, and P. J. Viccaro, Opt. Eng. **29**, 1273 (1990).

5. A. M. Khounsary, unpublished information, May1990, Patent application being filed 1991.

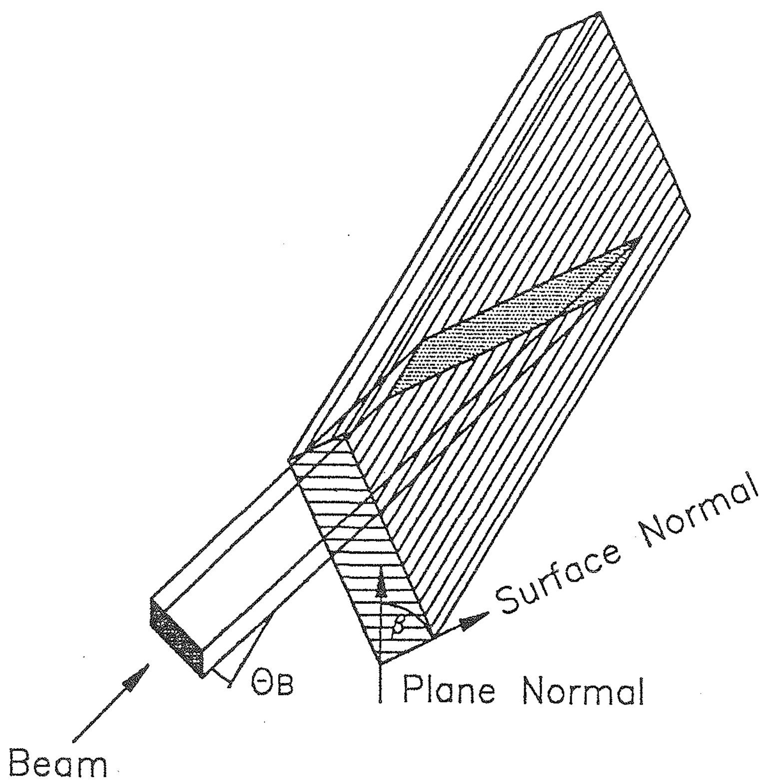


Fig. 1. A sketch of the inclined monochromator geometry and the conventional and inclined footprints. The crystal diffraction planes are shown. The inclination angle β is the angle between normal to the crystal surface and normal to the diffracting planes.

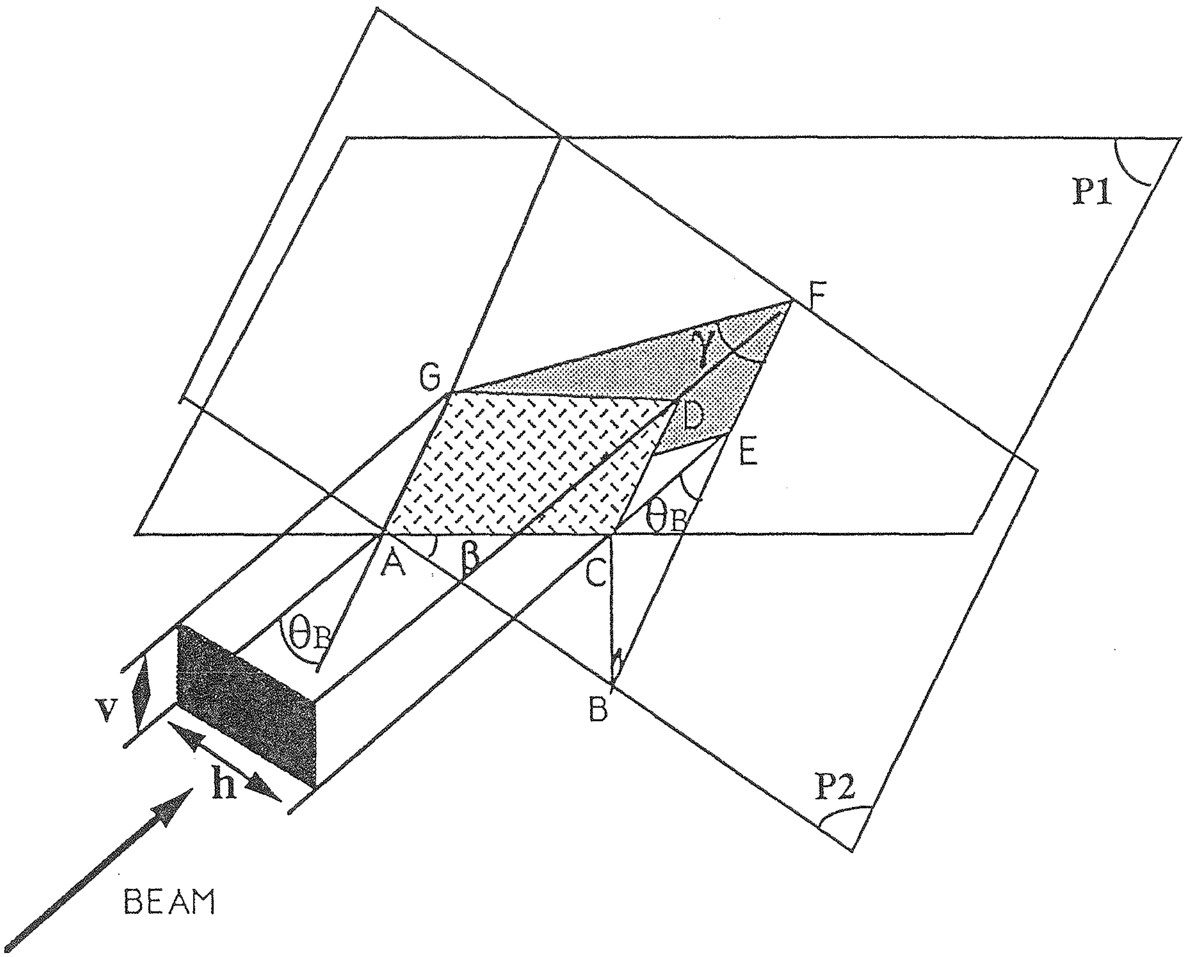
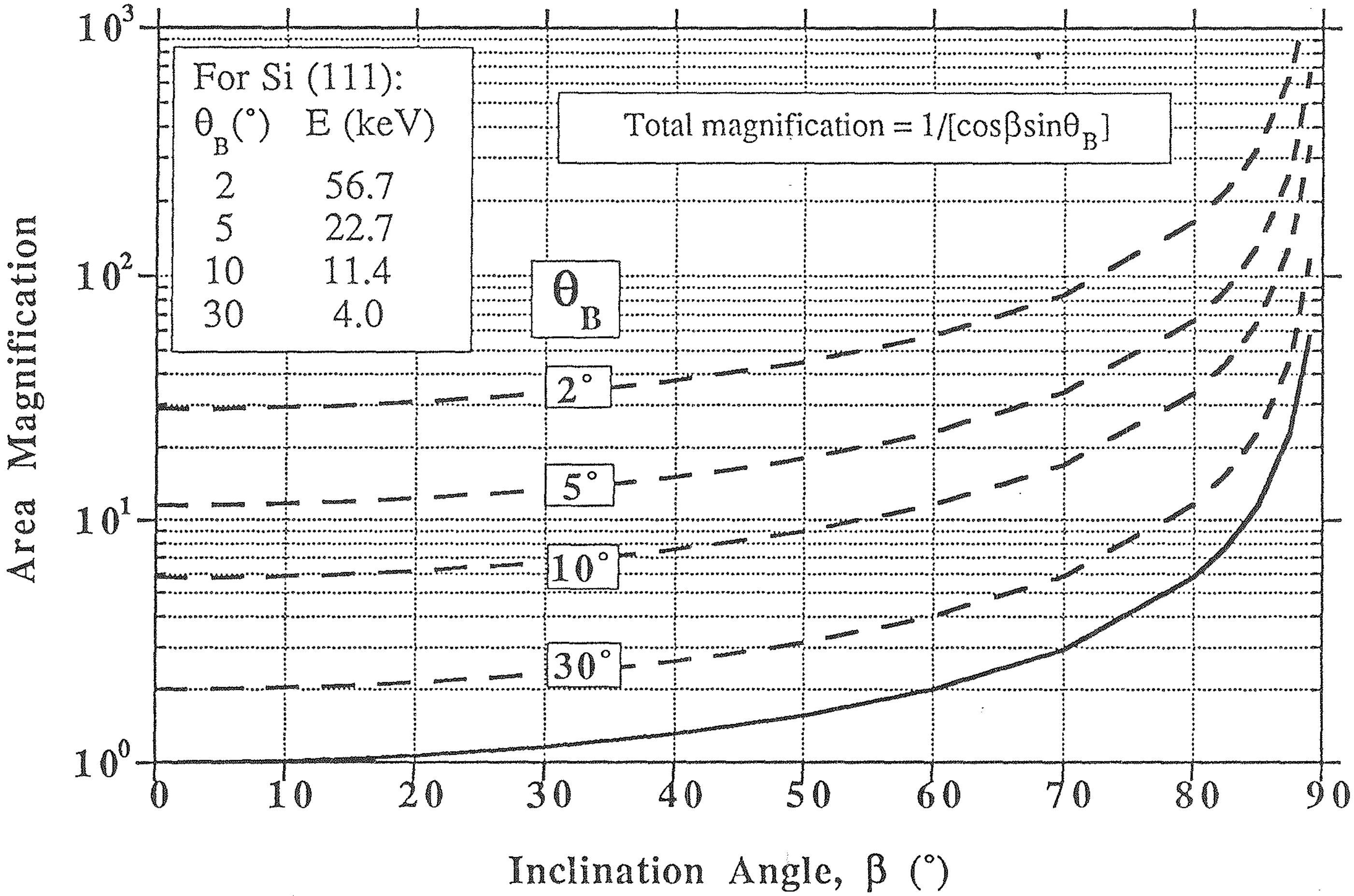


Fig. 2. A sketch of the footprints of a rectangular shaped beam on a conventional crystal (ACDG) and on an inclined crystal (AEFG).



Inclined Area Oct 90/data

Fig. 3. Magnigications of the beam footprint on an inclined crystal as a function of the inclination angle for a few Bragg angles (solid line). Shown in dotted lines are the magnifications as compared with the conventional monochromator footprint.

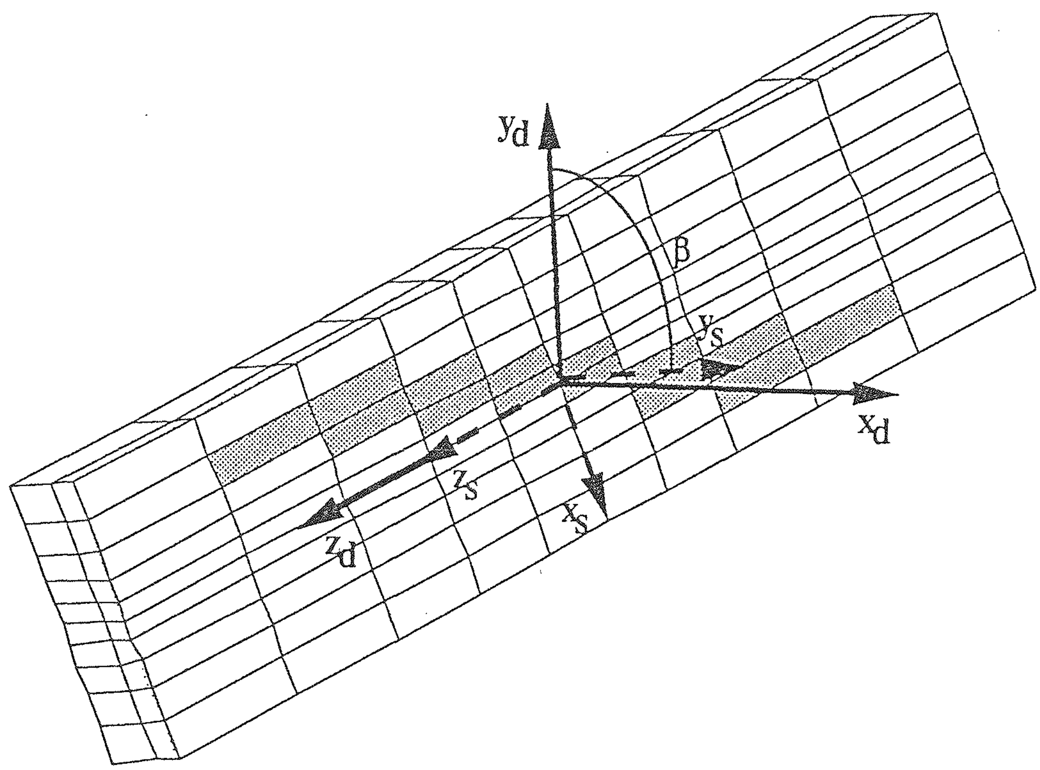


Fig. 4. A sketch of the model used in the numerical analyses. Also shown are two coordinate systems, one orthogonal with respect to the crystal surface ($x_s y_s z_s$) and the other orthogonal to the diffraction planes ($x_d y_d z_d$).

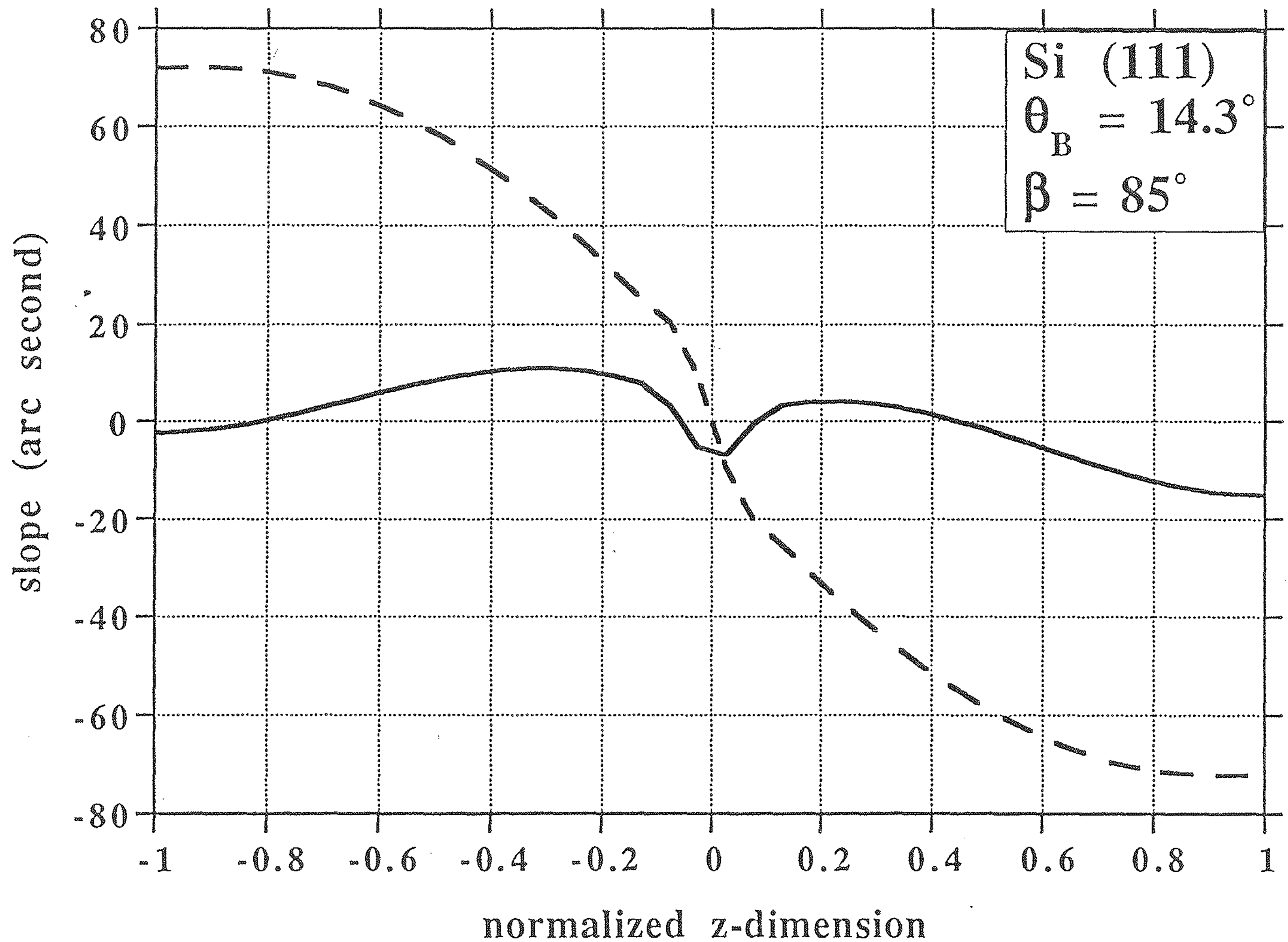


Fig. 5. The slope error profiles in the xy planes of the surface (dashed line) and diffraction (solid line) coordinate systems. Diffraction is from Si (111) for a Bragg angle of 14.3° (8 keV) and inclination angle of 85°.